# INCOMMENSURABILITY IN THE MAGNETIC EXCITATIONS OF THE BILINEAR-BIQUADRATIC SPIN-1 CHAIN

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(December 9, 1998)

We study the magnetic excitation spectrum of the spin-1 chain with Hamiltonian $\mathcal{H} = \sum_i \cos\theta \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin\theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$. We focus on the range $0 \leq \theta \leq +\pi/4$ where the spin chain is in the gapped Haldane phase. The excitation spectrum and static structure factor is studied using direct Lanczos diagonalization of small systems and density-matrix renormalization group techniques combined with the single-mode approximation. The magnon dispersion has a minimum at $k = \pi$ until a critical value $\theta_c = 0.38$ is reached at which the curvature (velocity) vanishes. Beyond this point, which is distinct from the VBS point and the Lifshitz point, the minimum lies at an incommensurate value that goes smoothly to $k = 2\pi/3$ when $\theta$ approaches $\pi/4$, the Lai-Sutherland point. The mode remains isolated from the other states : there is no evidence of spinon deconfinement before the point $\theta = +\pi/4$. These findings explain recent observation of the behavior of the magnetization curve $M \approx (H - H_c)^{1/4}$ for $\theta = \theta_c$.

PACS: 75.10.Jm, 75.20.Hr

## I. INTRODUCTION

It is now well known that one-dimensional spin-$S$ Heisenberg antiferromagnets (AF) have qualitatively different properties according to whether the spin value $S$ is integer or half-integer[1]. The existence of a singlet-triplet gap just above the ground state is clearly established[2–5] by numerical techniques for the S=1 and S=2 cases. Our physical understanding of these phenomena is based on the construction due to Affleck, Kennedy, Lieb and Tasaki[6] (AKLT). These authors were able to obtain explicitly the ground state of the following bilinear-biquadratic Hamiltonian :

$$\mathcal{H}_{aklt} = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2, \tag{1.1}$$

where $\mathbf{S}_i$ are quantum $S = 1$ spin operators living on a chain whose sites are indexed by $i$. To construct the ground state wavefunction of the Hamiltonian (1.1), each original $S = 1$ spin is written as two $S$=1/2 spins in a triplet state. Then the ground state is obtained by coupling into a singlet state all nearest-neighbor spins-1/2, thus forming a crystalline pattern of valence bonds. This state is called the valence-bond-solid state (VBS). It is in fact the unique ground-state and excitations have a gap which is known rigorously to be nonzero. Many results followed from the VBS picture. For example, it implies that there are free spins 1/2 at the end of an open chain[7]. This has been verified experimentally[8,9] by electron spin resonance on copper spins randomly introduced in the S=1 AF chain compound NENP. The bulk excitations are easily pictured : by breaking a singlet bond into a triplet one creates a local objet that move along the chain. This is only an approximate eigenstate but it has good overlap[10–13] with the first excited state which is a triplet, the "magnon", as predicted in the original derivation of Haldane[1].

This appealing picture is certainly correct for the Hamiltonian (1.1) but it remains to be understood how closely it applies to the standard Heisenberg exchange Hamiltonian for which the biquadratic coupling in Eq.(1.1) is zero. Initial studies[14] proposed the generalized family of models :

$$\mathcal{H}_\theta = \sum_i \cos\theta \, \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin\theta \, (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2. \tag{1.2}$$

This family includes the familiar Heisenberg model for $\theta = 0$ and the AKLT Hamiltonian for $\tan\theta_{VBS} = 1/3$. Since the gap does not go to zero in the interval $[0, \theta_{VBS}]$ it is likely that there is no phase transition and that the two

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limiting Hamiltonians $\theta = 0$ and $\theta = \theta_{VBS} \simeq 0.3218$ share the same physics. It is exactly the same line of arguments that justify the use of Laughlin wavefunctions to describe correlated states of electrons in the Fractional Quantum Hall Effect[15].

However, the AKLT point has special properties : for example the spin correlation functions have a spatial decay which is purely exponential, contrary to the Ornstein-Zernicke decay which is observed for the Heisenberg model. A study of the family of models (1.2) revealed that the AKLT point is a *disorder* point[16] beyond which short-range incommensurability appears in real space spin correlations[17]. Hence, it is at a boundary in some sense. The evolution of the spin excitations as a function of $\theta$ is the subject of the present paper. For $\theta = \pi/4$ it is known from the Bethe Ansatz[18,19] that the spectrum is gapless and that excitations form a continuum as in the case of the spin-1/2 AF chain. Near the Heisenberg point, it is known that there is an isolated branch of triplet excitations[20] that enter in a two-particle continuum for a wavevector $q \approx 0.3\pi$. In the neighborhood of $q = \pi$ the continuum is well above the isolated mode. This holds also for the AKLT Hamiltonian, as shown by Lanczos diagonalization[21]. Since there is no phase transition with zero gap between $\theta = 0$ and the Lai-Sutherland point $\theta = +\pi/4$, the common belief is that things evolve smoothly. This rather vague statement deserves however more scrutiny in view of the change of the spin correlations at the AKLT point[17]. An interesting issue is the fate of the Haldane triplet mode that should ultimately disappear in the spinon continuum for $\theta = \pi/4$. It has been speculated recently[22] that beyond the AKLT point $\theta > \theta_{VBS}$ the Haldane mode disappears and is replaced instead by a gapped spinon continuum which becomes gapless only right at the Lai-Sutherland point. However this intriguing picture is based only on variational wavefunctions whose relevance to the problem is at least unclear. It has also been observed[23] that the magnetization curve $M(H)$ displays intriguing behavior for some value of $\theta$. Some recent work[24] has undertaken the study of dynamical properties between the Heisenberg and VBS points.

In this paper, we investigate the excitation spectrum for a range of values of $\theta$ in the Haldane phase. Our main finding is that the Haldane mode remains well-defined and isolated from other states : there is no deconfinement of spinons. The minimum wavevector of the dispersion relation $E(k)$ stays at the zone boundary $k = \pi$ till a critical value $\theta_c \approx 0.38$ which is *between* the $\theta_{VBS}$ and Lifshitz points[25] $\theta_L$ and clearly different from these two values. Beyond $\theta_c$ the dispersion has a minimum at some incommensurate wavevector that evolves smoothly towards $2\pi/3$ when $\theta \to \pi/4$. At $\theta_c$, the dispersion curve has a quartic minimum and we show that this implies a critical behavior $\approx (H - H_c)^{1/4}$ for the magnetization $M(H)$.

In sect. (II), we describe our results for the dispersion of the Haldane triplet obtained from Lanczos exact diagonalizations. In sect. (III), the single-mode approximation is applied to DMRG calculations of the static structure factor in order to estimate the lower edge of the excitation spectrum. We discuss the physical properties of the Haldane phase and the relationship with the nonlinear sigma model in sect. (IV). We discuss also the shape of the magnetization curve in sect. (IV). Finally our conclusions are presented in sect. (V)

## II. LANCZOS RESULTS

At the Heisenberg point $\theta = 0$, the excitation spectrum of the hamiltonian (1.2) has been studied in considerable detail. We first use the Lanczos diagonalization method to study the interval $0 \leq \theta < +\pi/4$. We use conservation of the z-component of the total spin and compute the eigenenergies of the first 10 low-lying states. We use also translation symmetry to work in sectors with fixed lattice momentum $k$. To keep the hamiltonian real even when the momentum $k$ is not 0 or $\pi$, we use a non-trivial change of basis due to Takahashi[26]. This requires up to 350 Lanczos iterations which is considerably more expensive than just getting the ground state of each $S^z$ sector. To prevent runaway of the Lanczos process we are forced to re-orthogonalize with respect to the previous basis vector at each step. This bottleneck leads to a limit on the length of the chain which is 16 sites. This is a difficulty which does not appear when computing only the ground state. Our results for $\theta = 0$ are shown in Figure 1. Above the ground state, there is a well-defined triplet branch which is the prominent Haldane mode, the "magnon". The minimum of the dispersion is at the zone boundary $k = \pi$. This is the Haldane gap. The mode enters a continuum[20] at $k \approx 0.3\pi$. At $k = 0$ the continuum is the bottom of the spectrum and starts at twice the Haldane gap (approximately for N=16 sites on our figure but checked with excellent precision).

There is a nonzero curvature of the dispersion $E(k)$ at $k = \pi$. We model the bottom of the dispersion relation by a relativistic formula as suggested by the nonlinear sigma model :

$$E(k) = \sqrt{\Delta^2 + v^2(k - k_0)^2}. \tag{2.1}$$

Here $k_0$ is wavevector of the minimum, $\Delta$ is the gap and $v$ is the velocity. Close to the minimum we have :

$$E(k) \approx \Delta + \frac{v^2}{2\Delta}(k - k_0)^2. \tag{2.2}$$

The second derivative of the dispersion is thus simply related to the velocity that occurs in the nonlinear sigma model description.

When we increase $\theta$, there is a range of values for which nothing qualitatively new happens. This range *includes* the VBS point $\theta = \theta_{VBS} \simeq 0.3218$. The spectrum at this point is displayed in Figure 2. It shows the same features as that of Figure 1. Notably there is still a nonzero curvature at $k = \pi$ of the magnon branch. If we consider the energy of the state at $k_0 = \pi$ and the two closest states on the magnon branch with $k = \pi - 2\pi/N$ and $k = \pi - 4\pi/N$, we can fit by a fourth-order polynomial :

$$E(k) = E(k_0) + \frac{c}{2}(k - k_0)^2 + \frac{d}{24}(k - k_0)^4. \tag{2.3}$$

and hence obtain an estimate of the velocity. Close to the VBS point, the values of $c$ as a function of the chain length are given in Figure 3. At this point it is important to note that the finite-size effects are in fact extraordinarily small. This is related to the fact that the spin-spin correlations in the VBS wavefunction are of very short range $\xi = 1/\log 3 \approx 0.9$. So our estimate for $c$ is very precise : from N=4 to N=16 sites the dependence is very weak. We can exclude a vanishing velocity at this point. Indeed we find $c = 0.9778(1)$. Similarly the Haldane mode stays isolated from the continuum which lies much above : these states display extremely fast convergence to the thermodynamic limit.

We observe in Figure 3 that the velocity vanishes at a point $\theta_c = 0.38$ which is between the VBS point $\theta_{VBS} = 0.32$ and the Lifshitz point $\theta_L = 0.414$. There the minimum of the dispersion relation becomes of fourth order but still there are no states coming from above to fill the gap between the Haldane mode and the continuum. This case is shown in Figure 4. Once again we are in a regime of very weak finite-size effects : measurements of the spin correlation in this regime[17] are in agreement with the present findings.

We can also obtain an estimate of the fourth derivative $d$ of the dispersion relation $E(k)$ through Eq. (2.3). It is given in the neighborhood of the VBS point in Figure 5. The size dependence is minimal again at $\theta_{VBS}$. Note that right at $\theta_c$ the fourth derivative $d$ clearly extrapolate to a positive non-zero value : this fact will be important to explain the shape of the magnetization curve in sect.(IV).

Beyond the special point $\theta_c$, the minimum of the dispersion no longer lies at $k = \pi$ but is at a wavevector which is in general incommensurate and dependent upon $\theta$. The curvature of the dispersion is now negative at the zone boundary : see Figure 3. A typical case is shown in Figure 6 for $\theta = 0.52$. There is no evidence for the deconfined spinons proposed by Yamamoto[22]. If this was the case, the corresponding energy states should be filling the empty interval above the Haldane triplet mode. We see no evidence for this.

When $\theta \to \pi/4$ the gap closes and the overall picture is consistent with the apparition of the tripled period $2\pi/3$. However in this regime finite-size effects become important as the phase transition is approached. It is known that right at the Lai-Sutherland point, the phase transition is described by a a SU(3) generalization of the Kosterlitz-Thouless phase transition[27] For $\theta > \pi/4$, the system enters a gapless phase. In the regime $-\pi/4 < \theta < \pi/4$, it is extremely likely that the gap vanishes only at $\theta = \pm\pi/4$[17,12]. However, we cannot exclude from our numerical study that spinon deconfinement appears before that point but this would involve yet another phase transition for which there is at the present time no evidence.

## III. SINGLE-MODE APPROXIMATION

To confirm the results obtained in the previous section, we now turn to the single-mode approximation of the dispersion relation. This approximation was introduced originally by Bijl and Feynman to determine the phonon-roton dispersion in superfluid $^4$He. It has been also successfully applied to Haldane gap systems[11].

The dynamical structure factor of the spin system is defined by :

$$S(q, \omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \sum_n e^{iqn} \langle S_n^\alpha(t) S_0^\alpha \rangle. \tag{3.1}$$

In this equation, the $\alpha$ index need not be specified since we consider only isotropic systems. The equal-time correlation function is :

$$S(q) = \langle S_q^\alpha S_{-q}^\alpha \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega S(q, \omega), \tag{3.2}$$

where $S_q^\alpha = 1/\sqrt{L} \sum_n e^{iqn} S_n^\alpha$. Imagine that we know the ground state $|0\rangle$. Then a guess for the first excited state may be simply $S_q^\alpha|0\rangle$. This is a triplet with lattice momentum $q$. This will be close to an exact excited state if the

dynamical structure factor $S(q,\omega)$ is strongly peaked at the energy $\omega_{SMA}(q)$ of the state $S^{\alpha}_{q}|0\rangle$. This energy is given by the formula :

$$\omega_{SMA}(q) = \frac{1}{2\,S(q)}\langle\left[S^{\alpha}_{-q},\left[\mathcal{H}_\theta, S^{\alpha}_{q}\right]\right]\rangle, \tag{3.3}$$

where $\mathcal{H}_\theta$ is the Hamiltonian. The advantage of the single-mode approximation is that it does not require a full dynamical study of the system : in Eq.(3.3), it is possible to evaluate all quantities once we have a good approximation for the ground state. This is feasible by the DMRG algorithm which is extremely efficient in quantum spin chains. The commutators in Eq.(3.3) can be evaluated straightforwardly with the result :

$$\omega_{SMA}(q) = (\cos q - 1)c(\theta)/S(q), \tag{3.4}$$

where $c(\theta)$ is some constant given by :

$$\begin{aligned} c^{x}(\theta) = \cos\theta\left[< S^{y}_{i}S^{y}_{i+1} > + < S^{z}_{i}S^{z}_{i+1} >\right] + \sin\theta[2 < (\vec{S}_i\cdot\vec{S}_{i+1})^2 > - < (\vec{S}_i\cdot\vec{S}_{i+1})S^{x}_{i}S^{x}_{i+1} + S^{x}_{i}S^{x}_{i+1}(\vec{S}_i\cdot\vec{S}_{i+1}) > \\ + 2 < S^{y}_{i}S^{z}_{i}S^{z}_{i+1}S^{y}_{i+1} + S^{z}_{i}S^{y}_{i}S^{y}_{i+1}S^{z}_{i+1} > -2 < (S^{z}_{i})^2(S^{y}_{i+1})^2 + (S^{y}_{i})^2(S^{z}_{i+1})^2 >]. \end{aligned} \tag{3.5}$$

We find that $c(\theta)$ only varies slowly with $\theta$ and it is now obvious that at least within the single-mode approximation the minimum in $\omega(q)$ will start to move away from $\pi$ before the Lifshitz point is reached (at the Lifshitz point the maximum of $S(q)$ moves away from $\pi$). At the VBS point the ground state $|VBS\rangle$ is simple enough that $\omega_{SMA}(k)$ can be calculated exactly[11]. One has $\omega_{SMA}(k) = \frac{\sqrt{5}}{9\sqrt{2}}(5+3\cos k)$. Hence, we see explicitly that at the VBS point the second derivative and hence the velocity is non-zero within the SMA approximation. The value of the second derivative $c_{SMA} = 1.054$ is very close to our Lanczos estimate of sect. II $c = 0.9778$.

Using the above expressions, $c(\theta)$ as well as $S(q)$ have been calculated with the DMRG. We present results in the interval between $\theta_c$ as defined in sect.(II) and $\theta_L$. In Figure 7, the structure factor is plotted in the neighborhood of the zone boundary $q=\pi$. It becomes very flat, i.e. of fourth order at the Lifshitz point $\theta_L \simeq 0.414$. However, the minimum in $\omega_{SMA}(q)$ starts to move away from $\pi$ for $\theta \in [0.38, 0.39]$ : this can be seen on Figure 8 where this quantity is plotted close to $q=\pi$. This is consistent with our findings from the exact diagonalization results. Clearly, $\theta_c$ and $\theta_L$ are distinct, and in fact a considerable interval occurs between these two points.

Inherently the SMA approximation assumes that

$$S(k,\omega) = S(k)\delta(\omega - E(k))$$

and hence neglects any incoherent background. Thus, $\omega_{SMA}(k)$ *always* over estimates the true excitations. This is important to remember when one compares the SMA results for the gap with other numerical estimates. Roughly the distance that the SMA value is above the true gap measures how big the incoherent contribution to $S(k,\omega)$ is. It works quite well around the Lifshitz point.

## IV. STRUCTURES WITHIN THE HALDANE PHASE AND MAGNETIZATION PROCESS

From the numerical studies, both Lanczos and DMRG for single-mode approximation, we obtain a rather intricate structure within the Haldane phase $-\pi/4 < \theta < +\pi/4$.

• In the interval $-\pi/4 < \theta \leq \theta_{VBS}$, the dispersion relation has its minimum at $k=\pi$, the spin correlations are commensurate : $\langle \mathbf{S}_0\cdot\mathbf{S}_x\rangle \simeq (-)^x \exp(-x/\xi)/\sqrt{x}$. In this regime the O(3) non-linear sigma model is a perfectly correct description of the low-energy long-wavelength behavior of the system in agreement with the original derivation by Haldane[1].

• In the interval $\theta_{VBS} < \theta \leq \theta_c$, the dispersion relation still has its minimum at $k=\pi$ but now the spin correlations oscillate with a period which is incommensurate[17], This is not seen in the static structure factor S(q) which remains peaked at $q=\pi$, a feature due to the short-range nature of the spin order. While $E(k)$ is still sigma model like, this regime is *not* described by the sigma model which has only commensurate spin correlations. Indeed the nonlinear sigma model uses the Ansatz :

$$\mathbf{S}_i = (-)^i\phi_{\mathbf{i}} + \mathbf{L}_{\mathbf{i}}, \tag{4.1}$$

where the fields $\phi$ and $\mathbf{L}$ are smooth i.e. have Fourier modes only near $k=0$. This is no longer valid even without a phase transition as a function of $\theta$.

• In the interval $\theta_c < \theta \leq \theta_L$, the dispersion has now a minimum away from the zone boundary. In fact there are two nonequivalent wavevectors $\pi \pm Q$ at the minimum. The quantity S(q) is still peaked at $q = \pi$. A possible effective theory would be now a non-linear sigma model describing helical order[28,29]. It would involve a $3 \times 3$ rotation matrix as an order parameter to describe the short-range spin order. It is a phase with incommensurate short-range spin correlations and the spinon are *confined*.

• In the interval $\theta_L < \theta \leq +\pi/4$, the only difference with the previous case is that there is a double-peak structure in S(q).

The above observations have interesting consequences for the magnetization curve M(H). For the Heisenberg model, its shape and essential characteristics are well understood[30,3]. When the applied uniform magnetic field H is less than the Haldane gap, there is no net magnetization : since H is coupled to the z-component of the total spin, the Zeeman Hamiltonian commutes with the Heisenberg Hamiltonian and hence does not change wavefunctions. So the ground state is unaffected by H. However at a critical value $H_{c1} = \Delta$, the Haldane gap, there is a crossing of levels and a magnetized state becomes the ground state. Finally there is full saturation to a ferromagnetic state beyond some field $H_{c2}$. Near $H_{c1}$, the critical behavior is given by $M(H) \simeq (H - H_{c1})^{1/2}$. The exponent 1/2 is directly related to the dispersion relation of the magnons near $k = \pi$. Indeed the magnetization is given by inverting the relation $H - H_{c1} = dE/dM$ and the function E(M) is the same as for a system of noninteracting fermions :

$$E = (\Delta - H)M + N \int_{-k_F}^{+k_F} \frac{dk}{2\pi} \frac{v^2 k^2}{2\Delta}. \tag{4.2}$$

In this equation, N is the number of sites and $v$ is the velocity which is defined through the dispersion relation :

$$E(k) = \Delta + \frac{v^2}{2\Delta}(k-\pi)^2 + c_4(k-\pi)^4 + O(k-\pi)^6. \tag{4.3}$$

Since $M = Nk_F/\pi$, one has :

$$E(M) = M(\Delta - H) + \frac{(v\pi)^2}{6\Delta}\frac{M^3}{L^2} + d_4 M^5 + O(M^7). \tag{4.4}$$

Near the critical field this leads to $M \simeq (H-\Delta)^{1/2}$. This depends crucially on the quadratic dispersion relation. If now we consider the generalized Hamiltonian at $\theta = \theta_c$, one has $v = 0$ but the fourth-order derivative is nonzero as can be seen in Figure 5. Hence Eq.(4.3) should be replaced by $E(k) = \Delta + c_4(k-\pi)^4$. There is no cubic term by imposing invariance under $k \to 2\pi - k$ which is parity and lattice periodicity. Now in Eq.(4.4), the $M^4$ term dominates and this leads immediately to $M \simeq (H-\Delta)^{1/4}$. Our findings explain the observation of such a behavior by Okunishi et al.[23]. When $\theta > \theta_c$ the dispersion has again a *quadratic* minimum and the line of arguments with $v \neq 0$ is again valid : $M \simeq (H-\Delta)^{1/2}$ is the correct behavior in this range. The massless phase above $H_{c1}$ however is likely to be[31] a two-component Luttinger liquid, contrary to the one-component Luttinger liquid that arises for $\theta < \theta_c$.

## V. CONCLUSION

We have studied the magnetic excitation spectrum of the bilinear-biquadratic S=1 Hamiltonian that includes the Heisenberg point as well as the VBS point. We have shown by Lanczos and DMRG techniques combined with the single-mode approximation that the magnon dispersion becomes incommensurate at a critical value $\theta_c = 0.38$ which is different from all previously known points in the phase diagram. Right at the special value $\theta_c$ the magnon dispersion has a fourth-order minimum at the zone boundary $k = \pi$. As a consequence the magnetization curve $M(H)$ near the lower critical field is drastically modified : instead of a square-root behavior, the magnetization rises with a power-law 1/4. This explains recent observations.

From our study it is now clear that there are hidden structures within the bulk of the Haldane phase. This phase extends in the interval $-\pi/4 < \theta < +\pi/4$ and the gap vanishes at the two boundary points. These critical points correspond, as is well known, to transitions towards completely different phases. It is widely believed that absence of phase transition means that the physics evolves smoothly, hence, that the Heisenberg point $\theta = 0$ and the AKLT point $\theta = 0.32$ share the same physical properties. It was known that spin correlations do change qualitatively even within the Haldane range $-\pi/4 < \theta < +\pi/4$. We have shown that also the dynamical properties do change qualitatively and not only quantitatively. Curiously enough the special point characterizing the change $\theta_c$ is distinct from the VBS point. The bilinear-biquadratic S=1 chain is thus an interesting counterexample showing the variety of physical phenomena that occur within a massive phase.

Finally we have shown evidence that there is no spinon deconfinement when we approach the SU(3) phase transition at $\theta = +\pi/4$. Thus, the Haldane phase is an example of a gapped spin liquid with incommensurate spin excitations, a phenomenon that may also appear in the normal phase of the underdoped cuprates.

**ACKNOWLEDGMENTS**

We thank G. Fáth and T. Garel for useful discussions, and IDRIS (Orsay) for allocation of CPU time on the C94 and C98 CRAY supercomputers and rs6000 workstations.

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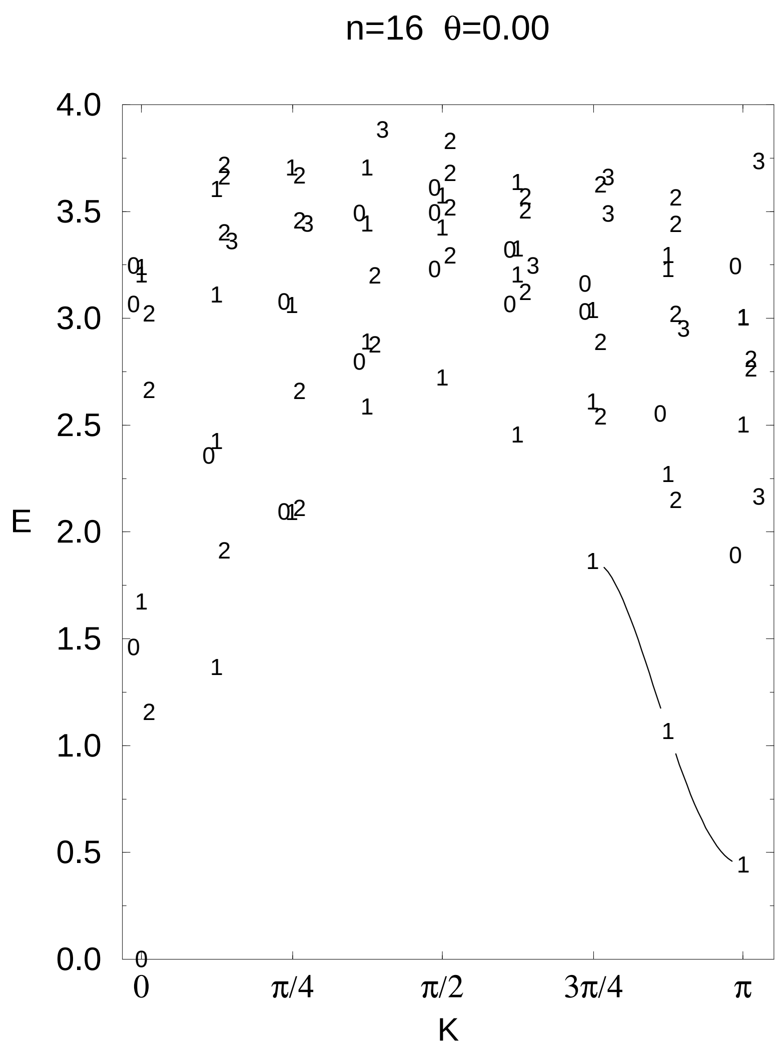


FIG. 1. Excitation spectrum of the N=16 chain for the Heisenberg S=1 AF chain, $\theta = 0$. Energies are relative to the ground state. The number denote the total spin value of each state. We have introduced small horizontal shifts to avoid superposition of symbols. The energies are given as a function of the chain momentum $k$ (only the first 10 levels are calculated for each momentum and $S^z$). Note the prominent triplet branch that starts from the Haldane gap at the zone boundary at $k = \pi$. The solid curve is the fit by Eq. (2.3).

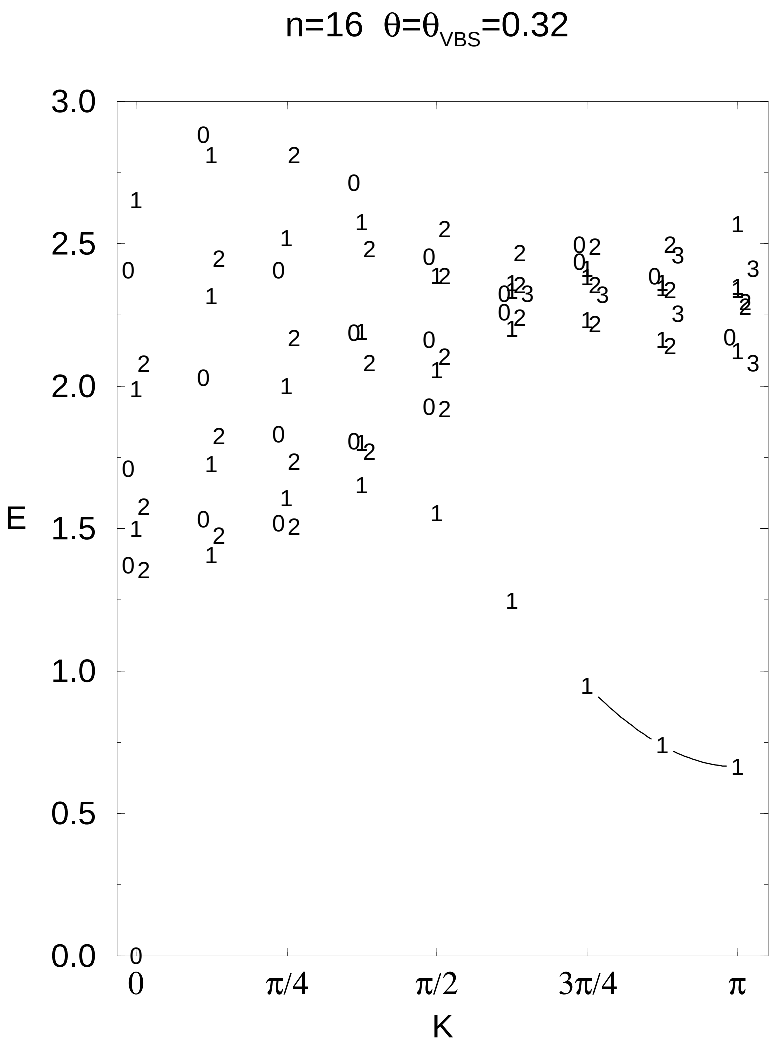


FIG. 2. Excitation spectrum of the N=16 chain for $\theta = \theta_{VBS}$. The physics is qualitatively similar to $\theta = 0$, there is evidence for a nonzero curvature of the dispersion at $k = \pi$ of the magnon and there is no spinon continuum.

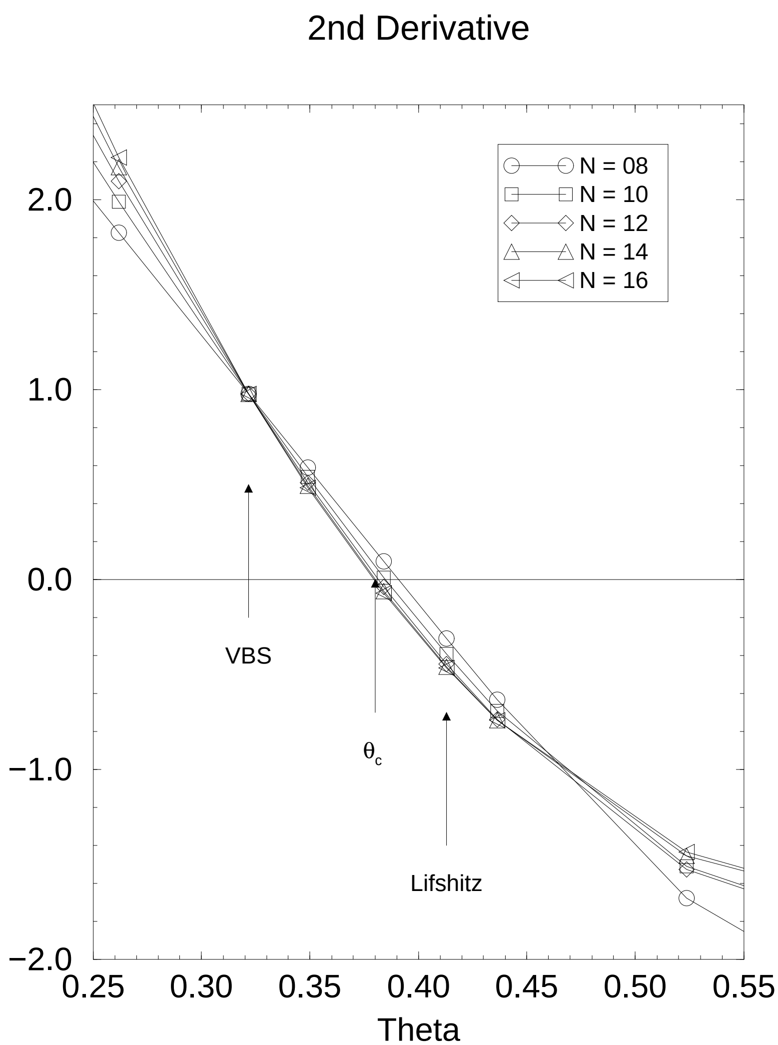


FIG. 3. The second derivative $c$ of the dispersion relation computed with the triplet state at $k = \pi$ and its two closest neighbors along the magnon branch. Data are for several sizes N=8,10,12,14,16. It is nonzero at the VBS point but vanishes for $\theta_c = 0.38$. Note that finite-size effects are extremely small in this range. We find $c_{VBS} = 0.9778(1)$.

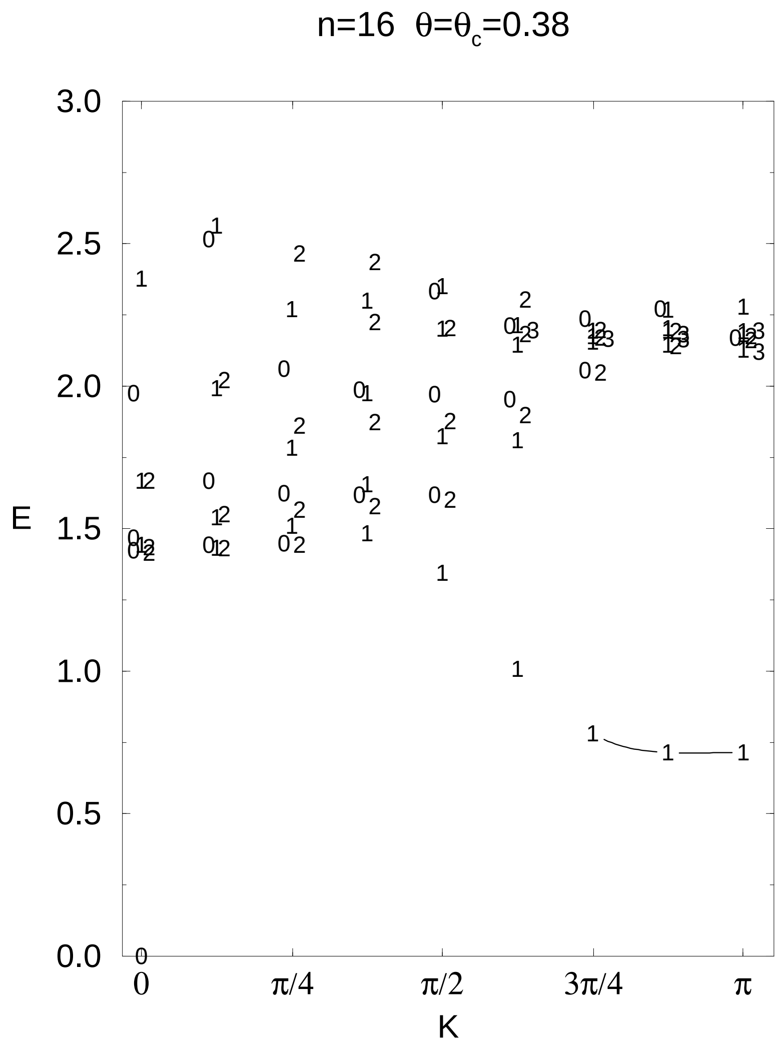


FIG. 4. Same spectrum as figure 1 but for $\theta = \theta_c$. At this point the dispersion of the triplet mode has a fourth-order minimum at the zone boundary.

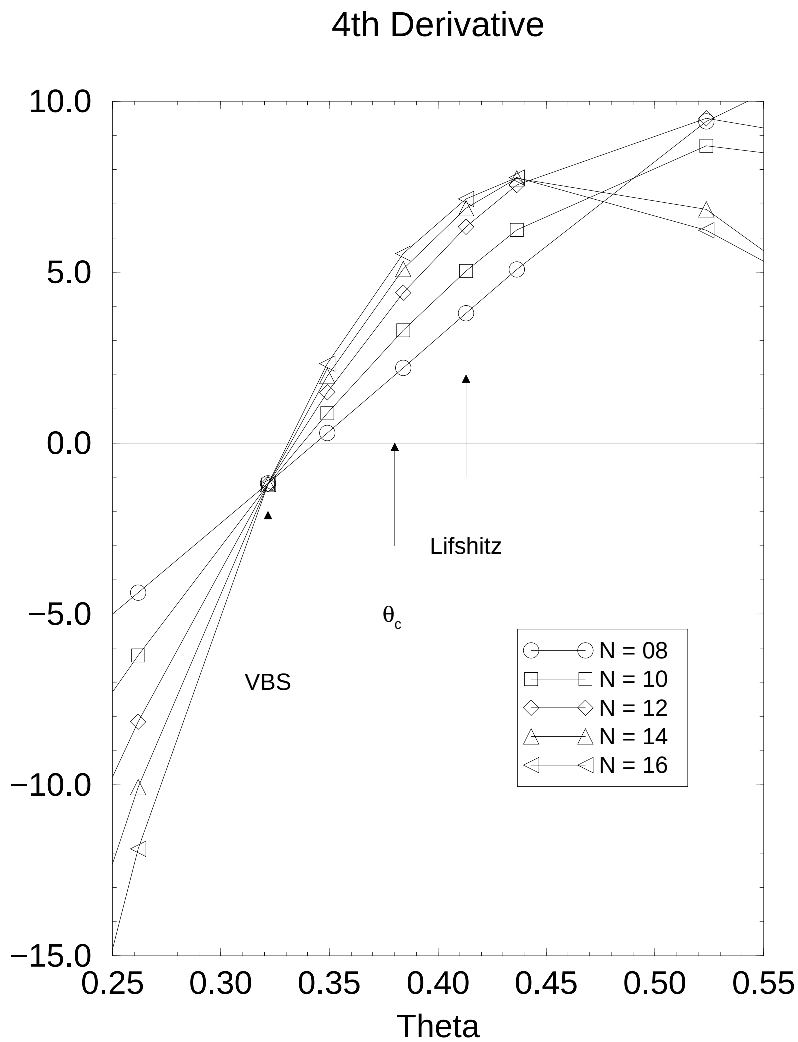


FIG. 5. The fourth-order derivative $d$ of the dispersion relation evaluated as in fig.(3) with the two closest neighbors. It is nonzero at $\theta_c$.

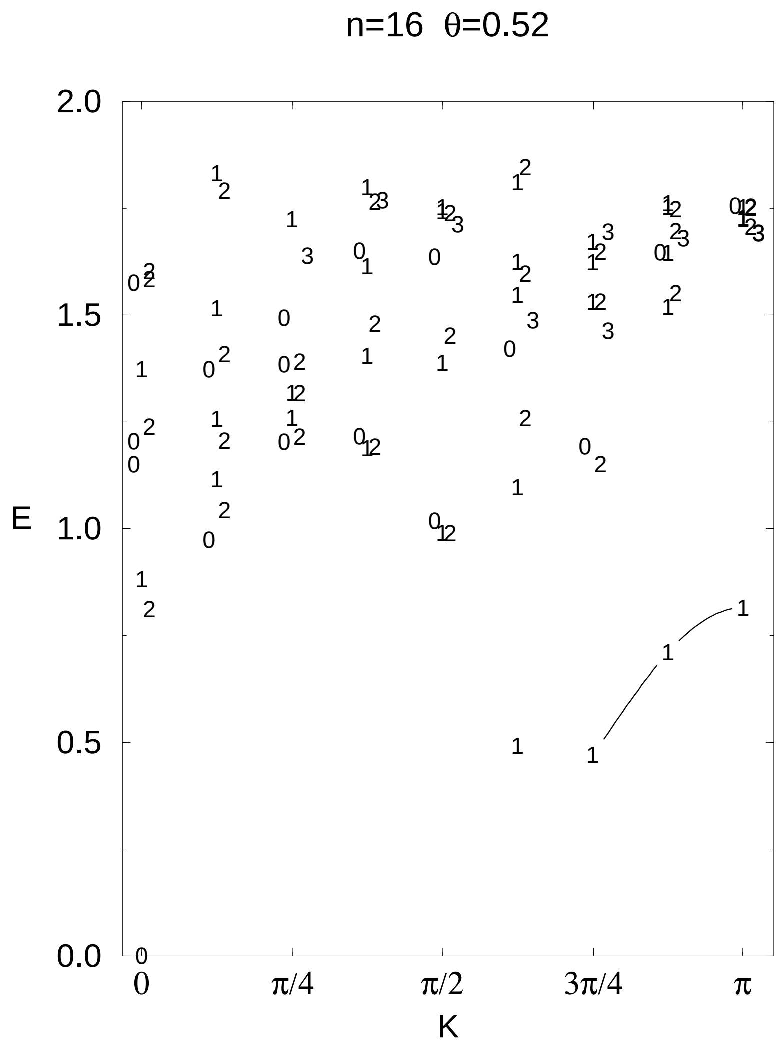


FIG. 6. Same spectrum as figure 1 for $\theta = 0.52$. This point lies deep in the incommensurate regime. The minimum wavevector is now inside the Brillouin zone and the magnon mode remains isolated : there is no evidence for spinon deconfinement.

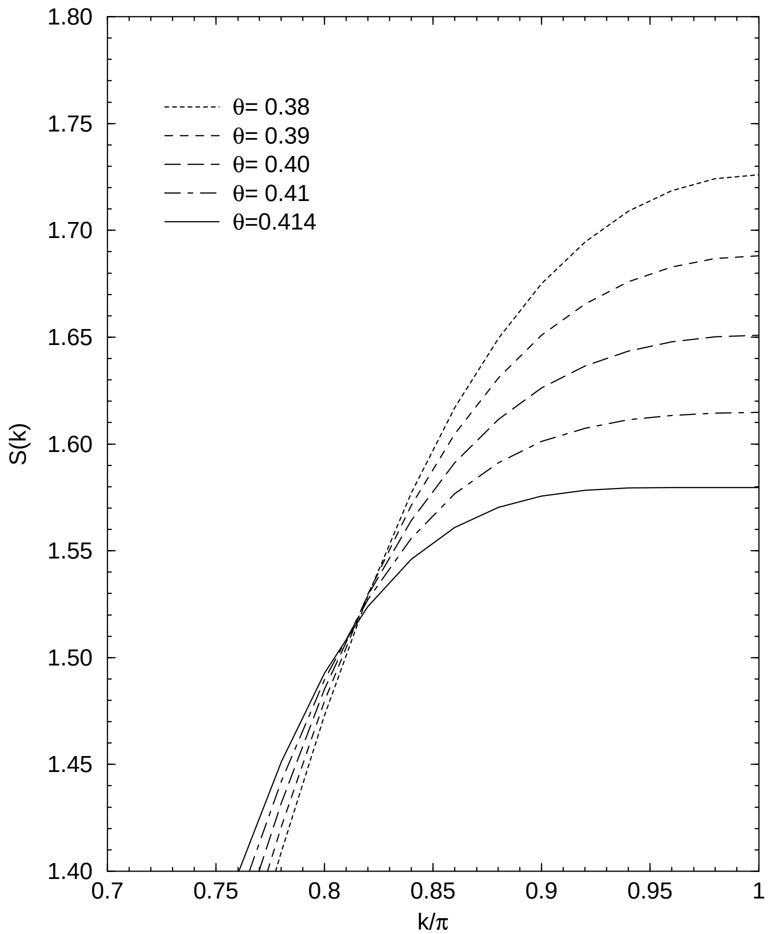


FIG. 7. The static structure factor from a DMRG calculation. It is drawn only near the zone boundary for several $\theta$ values in the interval $\theta_c, \theta_L$.

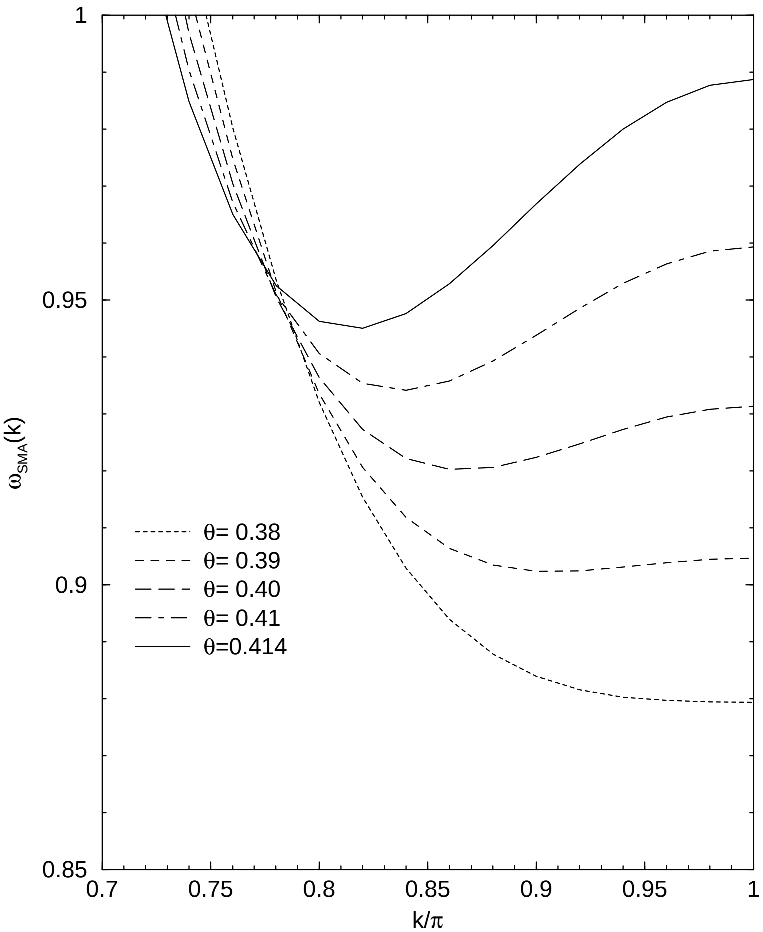


FIG. 8. The dispersion $\omega_{SMA}(k)$ obtained from the single-mode approximation. The minimum moves away from $k = \pi$ at the value $\theta_c$ which is the same as the Lanczos value 0.38(1). Energies have been divided by $\cos\theta$.